

2-D Model for CO₂ Leakage through a Fault with Multiphase and Non-Isothermal Effects—First-Generation Leakage Risk Profiles

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Cover Illustration: Diagram of simulated leakage scenario.

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2-D Model for CO₂ Leakage through a Fault with Multiphase and Non-Isothermal Effects—First-Generation Leakage Risk Profiles

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Acronyms and Abbreviations

Term	Description
1-D	One-dimensional
2-D	Two-dimensional
3-D	Three-dimensional
CO ₂	Carbon dioxide
LLNL	Lawrence Livermore National Laboratory
NRAP	National Risk Assessment Partnership
NUFT	Nonisothermal Unsaturated-Saturated Flow and Transport model
ROM	Reduced-order model
T-P	Temperature-pressure
UQ	Uncertainty quantification

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EXECUTIVE SUMMARY

Risk assessment methods are used to guide decision making during all phases of a carbon storage project, from initial site design and permitting all the way through shut-in and long-term maintenance. Unfortunately, significant science gaps exist in understanding the behavior of carbon dioxide (CO₂) storage reservoirs, leading to very large uncertainty bounds.

This work examines one key driver of risk: the potential for CO₂ and brine leakage out of a storage interval along a permeable fault zone considering multiphase and non-isothermal effects. Two key factors complicate this assessment and must be addressed: fault zones are known to exhibit very complicated multi-physics behavior, and direct characterization of the constitutive properties of a fault zone is typically unavailable.

A deterministic computational model is presented here for the behavior of a leaking fault connecting a CO₂ saline storage reservoir and a groundwater aquifer. Using a fluid flow simulator, Nonisothermal Unsaturated-Saturated Flow and Transport model (NUFT), 1,000 models were run varying five dimensions: fault permeability, aquifer permeability, scaling factor of caprock permeability, scaling factor of pressure, and scaling factor of distance. This deterministic model was then used within an uncertainty quantification (UQ) sampling framework in order to rigorously quantify the sensitivity of the output response to the input model parameters—that is, brine/CO₂ leakage rates as a function of the input constitutive properties and boundary conditions.

Response surfaces were constructed with PSUADE for 19 time steps from 0.5 to 1,000 years as functions of a refined parameter set. On each response surface, 100,000 models were run to generate CO₂ and brine leakage rate profiles for different percentiles. The response surfaces constitute a reduced-order model (ROM) that can be incorporated into a system model that predicts the potential for CO₂ or brine to be released from a storage reservoir to an overlying aquifer or the atmosphere (e.g., Pawar et al., 2013).

The current analysis corresponds to a first-generation of leakage risk profiles with the objective to provide leakage rates to the National Risk Assessment Partnership's (NRAP) Groundwater Protection Working Group. It has several assumptions and limitations mainly due to its two-dimensional (2-D) geometry and the simplistic representation of the fault zone geometry and properties. Furthermore, this model currently does not account for the effect of the in situ stress. All these limitations will be addressed in further stages of this work.

1. CONCEPTUAL MODEL

The fault leakage scenario described in this document corresponds to carbon dioxide (CO₂) and brine leakage through a fault that spans from a CO₂ storage reservoir in *Field A* to an overlying aquifer. The reservoir model of *Field A* is based on a real, large CO₂ injection site, currently in operation that has been history-matched with real wellbore and injection data.

Field A's reservoir (Figure 1) is a siliciclastic ~ 20-m thick unit at ~ 1,800-m depth. It is overlaid by a thick mudstone caprock, which in this model is ~ 1,500-m thick. Reservoir pressure, temperature, and saturation values are based on *Field A*'s reservoir model. However, aquifer characteristics, depth and thickness, as well as the fault, are hypothetical.

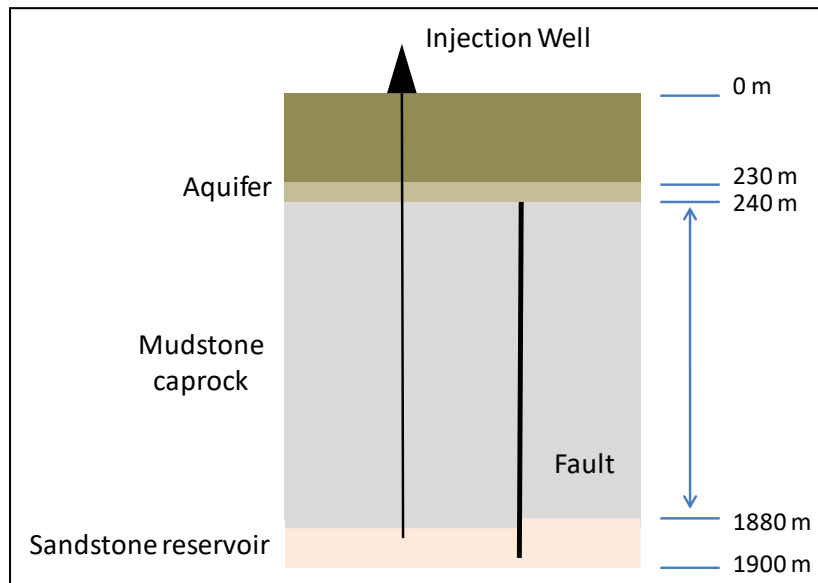


Figure 1: Diagram of simulated case, approximately based on *Field A*'s geology.

In the first-generation model, the following simplifications and assumptions were made. First the model is two-dimensional (2-D), which does not capture flow, pressure, and mass transport along the strike of the fault. Similarly, a 2-D model does not capture the interaction of a three-dimensional (3-D) CO₂ plume intersecting the fault plane. Furthermore, the fault is represented in a very simplistic way, as a single plane continuous all the way to the aquifer, with a single and constant value of permeability, as well as constant fault continuity and thickness. This model does not account for the fault structure, differential permeability perpendicular vs. parallel to the fault, heterogeneities along the fault, diagenesis or stress dependent permeability, nor the response of the fault to the in situ stress. These factors will be incorporated in future generations of risk profiles.

2. PARAMETER RANGE

In the literature examined, fault permeability has been estimated using a variety of approaches that incorporate deformation mechanism, host rock lithology, presence of clays, diagenesis, stress, etc. In this particular case, given the hypothetical nature of the fault, published relationships of fault permeability and host rock permeability for siliciclastic sediments were used (Antonellini and Aydin, 1994; Hippler, 1997; Fisher and Knipe, 1998) (Table 1). Similarly for caprock permeability and aquifer permeability, published values of common caprocks were used (Birkholzer et al., 2009; Preisig and Prevost, 2011).

Table 1: Parameters used during base case simulations and range of uncertainty of those properties used during the uncertainty quantification (UQ) analysis

Parameter	Base Case	Uncertainty Range
Fault permeability [m ²]	10 ⁻¹³	10 ⁻¹⁹ to 10 ⁻¹³
Caprock permeability [m ²]	10 ⁻¹⁹	10 ⁻²¹ to 10 ⁻¹⁶
Aquifer permeability [m ²]	10 ⁻¹⁴	10 ⁻¹⁵ to 10 ⁻¹³
Fault porosity [%]	10	--
Aquifer porosity [%]	25	--
Fault thickness [m]	0.5	--
Specific heat capacity of caprock [J/kg/°C]	1,000	--
Saturated thermal conductivity [W/m/°C]	2.5	--

3. FLOW SIMULATION

The flow simulations presented in this document were performed with NUFT (Nonisothermal Unsaturated-Saturated Flow and Transport model). NUFT is a flexible multi-purpose computer code for modeling fluid flow and transport in porous media under both non-isothermal and isothermal conditions. It solves the continuum equations for the conservation of mass and energy.

When supercritical CO₂ migrates upward through the permeable fault, a phase change happens because of the decrease in temperature and pressure. The larger change of CO₂ density during this phase transition will make the temperature decrease, the so-called Joule-Thomson effect. The thermal effects make the process multi-dimensional even under idealized conditions where upflow would be confined to a vertical one-dimensional (1-D) channel with impermeable boundaries (Pruess, 2003). Here a 2-D model is established to model the fluid flow and heat transfer during the CO₂ leakage (see Figure 2). The leaking fault connects the storage reservoir to a groundwater aquifer. In the base case scenario, it is assumed that the caprock is relatively impermeable with isotropic permeability equal to 10^{-19} m² (Preisig and Prevost, 2011). The permeability of the vertical fault in the base case scenario is assumed to the largest value of the estimated range described in the previous section, 10^{-13} m². The permeability of aquifer is one magnitude smaller than that of fault (Pruess, 2003). The fault may exchange heat with the surrounding rock. The specific heat capacity of the caprock is set up to 1,000 J/kg/°C with a saturated thermal conductivity equal to 2.5 W/m/°C (Preisig and Prevost, 2011). The porosity of the fault is 0.1, and is 0.25 in the aquifer. Boundary conditions at the upper aquifer layer are a hydrostatic pressure $2.254 \cdot 10^6$ bars and a temperature at 21.9°C, which is calculated based on the assumption that the land surface temperature is 15°C with a geothermal gradient of 30°C/km. The temperature at the inlet of the fault is 95°C, which is same as *Field A*'s reservoir. Variable conditions are used for the pressure and liquid saturation at the inlet of fault (see Figures 2 and 3). These values are the outputs of pressure and brine saturation at the top layer and injection well location of *Field A*'s reservoir, which includes data during the CO₂ injection and also captures the pressure decrease when the injection stops.

Table 2: Boundary conditions of flow simulations

Location	Pressure [bars]	Temperature [°C]	Saturation
Upper aquifer layer	$2.254 \cdot 10^6$ (hydrostatic)	21.9	1
Inlet of fault	variable	95.0	variable

Prior to introducing CO₂ into the fault, an initial state is prepared to generate the pressure and temperature distribution in all domains. Then the model is run using the pressure and brine saturation history at the inlet boundary (see Figures 2 and 3). The model includes transitions between super- and sub-critical conditions, considers the non-linear CO₂ enthalpy functions given by Span and Wagner (1996) and the viscosity function given by Fenghour and Wakeham (1998). For numerical simulation the system is discretized into 99 layers with thickness varying from 1 m to 200 m. In the horizontal direction, 11 grid blocks are used, starting with 0.5 m for the fault. The simulation time is 1,000 years.

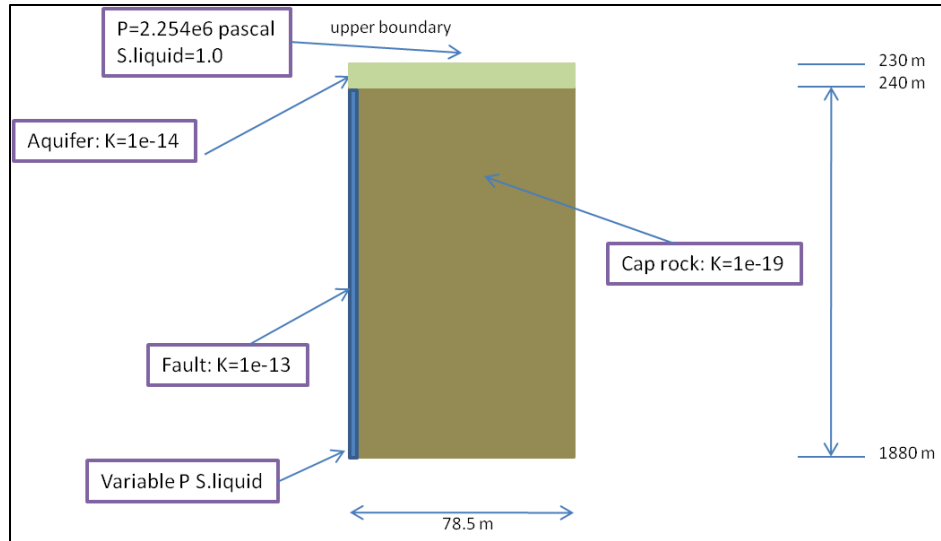


Figure 2: 2-D flow system.

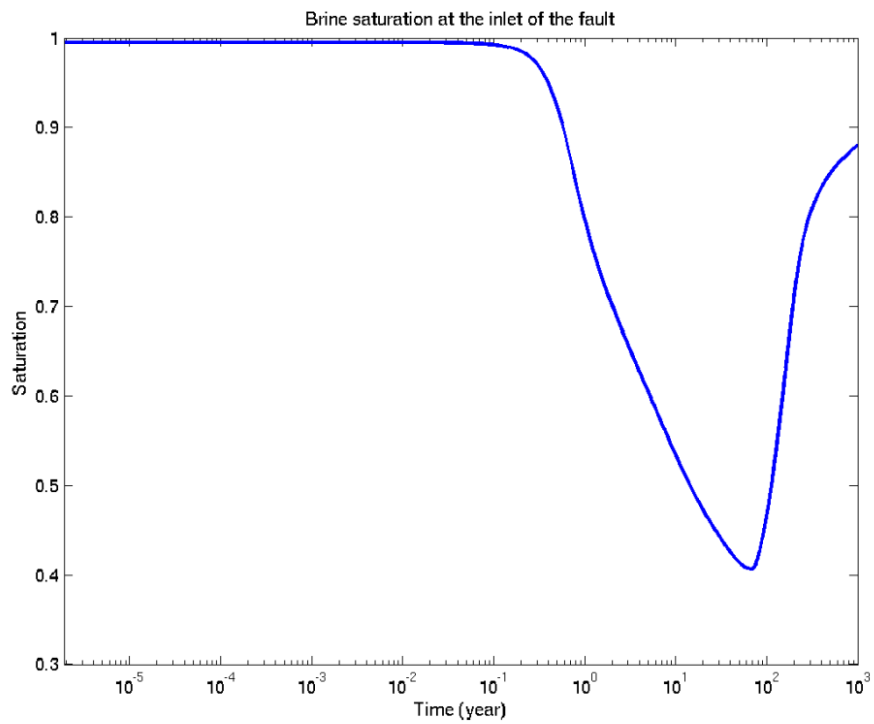


Figure 3: Brine saturation history at the inlet of fault.

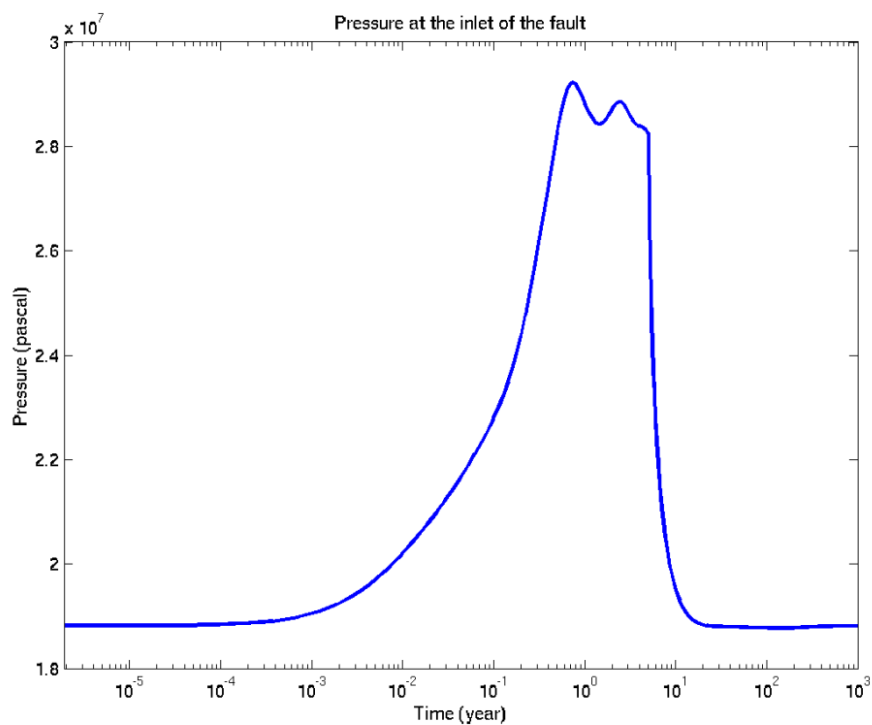


Figure 4: Pressure history at the inlet of fault.

4. RESULTS OF FLOW SIMULATION

During the period of CO₂ injection, the pressure in the reservoir is high. The pressure decreases when the injection stops at 5 years and to background hydrostatic pressure 20 years later. The high pressure in the reservoir causes the pressure in the fault to increase, such that the transition point of CO₂ from supercritical to gas is lower: 473 m at 1 year (see Figure 5). With the continuing decrease of pressure after 5 years, the depth of phase transition extends to more than 700 m, and is 773 m at 1,000 years (see Figure 5). The phase transition causes the decompression of gas-like subcritical CO₂, which comes with the heat sorption, the so-called Joule-Thomson effect. This non-isothermal effect can be seen clearly from Figures 5 and 6. The temperature – pressure (T-P) profile along the fault at 5 years approximately follows the CO₂ saturation line beyond the critical point. Temperature increases near the bottom of the overlying two-phase aqueous-gas zone, but resumes an enhanced decline due to Joule-Thomson cooling as the gas expands during upward flow (Pruess, 2011). The lower temperature gas accumulates in the aquifer; the temperature at the aquifer near the fault outlet boundary keeps decreasing before 100 years. But the lower temperature zone disappears 1,000 years later. When the overpressure in reservoir disappears, CO₂ leakage is only driven by buoyancy and the leakage rate decreases, the heat exchange between the fault and caprock makes the non-isothermal effect unclear.

At early time, outflow at the outlet of fault is only brine. A large water outflow occurs as free CO₂ approaches the outlet of fault (see Figure 7). The largest CO₂ flux approaches $4.1 \cdot 10^{-3}$ kg/s/m² when the injection stops at 5 years. The CO₂ flux rate decreases after 5 years and increases again later because of the continual accumulation of CO₂ in the reservoir (see Figure 3). The CO₂ flux rate reaches the second peak value at 150 years because the CO₂ saturation at the inlet remains large during this period. The CO₂ flux value continues to decrease 150 years later because the CO₂ saturation at the inlet keeps decreasing and there is no overpressure drive anymore. The decreasing CO₂ flux will cause the gas saturation in the outlet to decrease (see Figures 8 and 9). On the other hand, the brine saturation at the later part increases. Some water flows downward because of the decrease of CO₂ flux.

When the pressure is high, the density of CO₂ is also high (see Figure 10). At 1 year, the density change along the fault respects the phase change around 470 m clearly. Later on, the change of pressure is not so much (after 10 years); the density curve along the fault does not change drastically. The viscosity is a function of temperature and density, so the difference of CO₂ viscosity along the fault between 1 year and 10 years is bigger (see Figure 11). The general curve pattern is similar to that of CO₂ density.

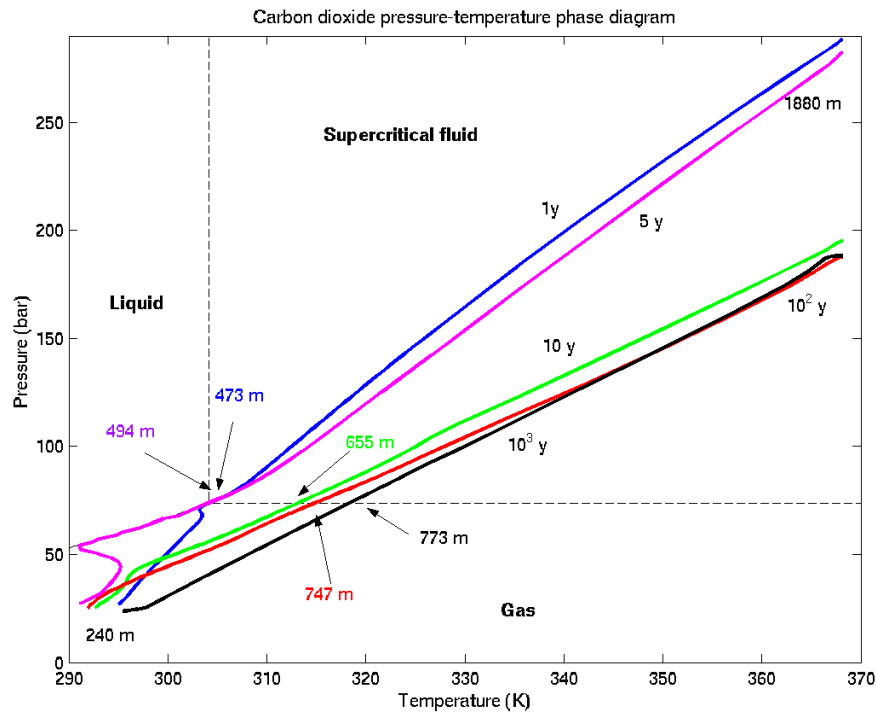


Figure 5: Temperature-pressure profiles along the fault at different times.

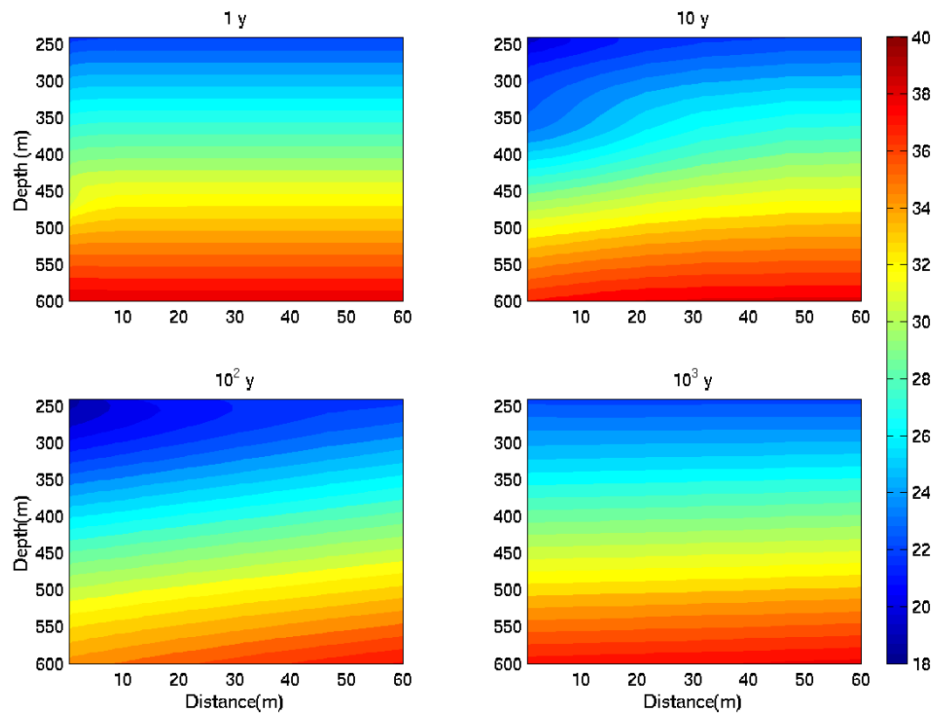


Figure 6: Temperature distribution at different times.

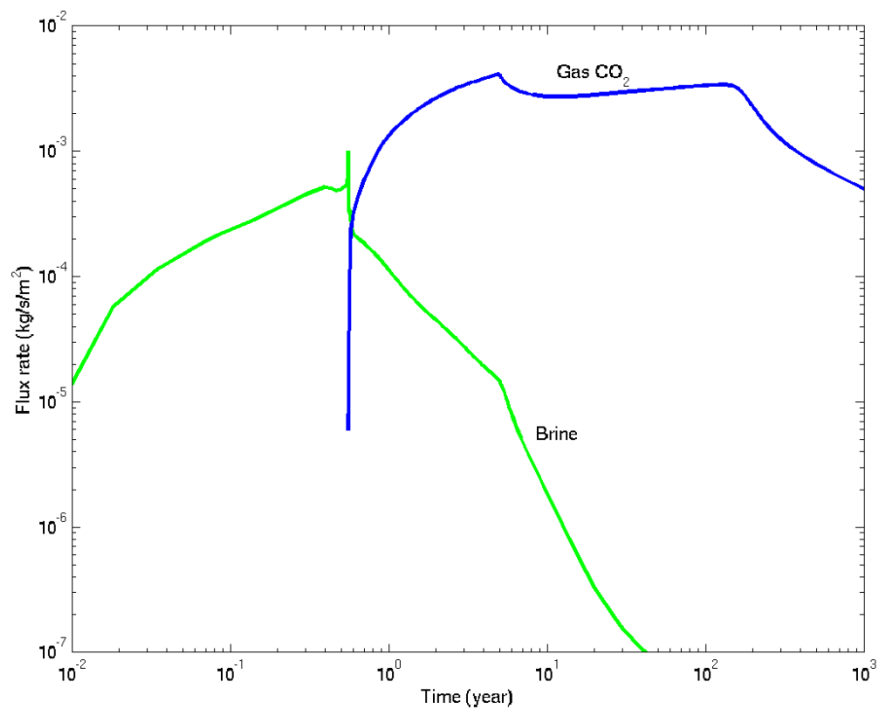


Figure 7: Flux rate of brine and gas CO₂ at the outlet of fault.

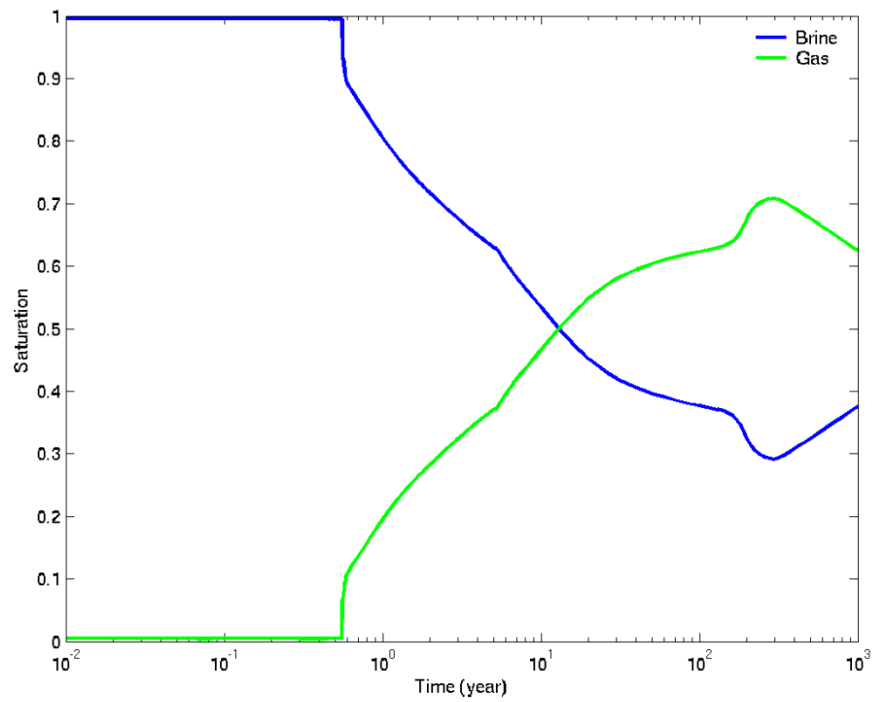


Figure 8: Saturation evolution at the outlet of fault.

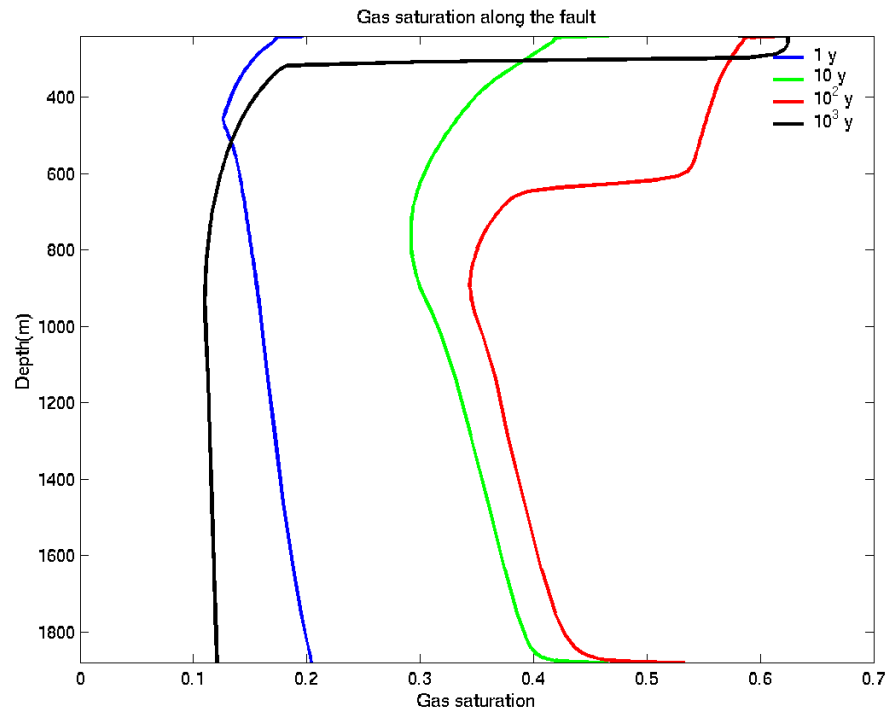


Figure 9: Gas saturation along the fault at different times.

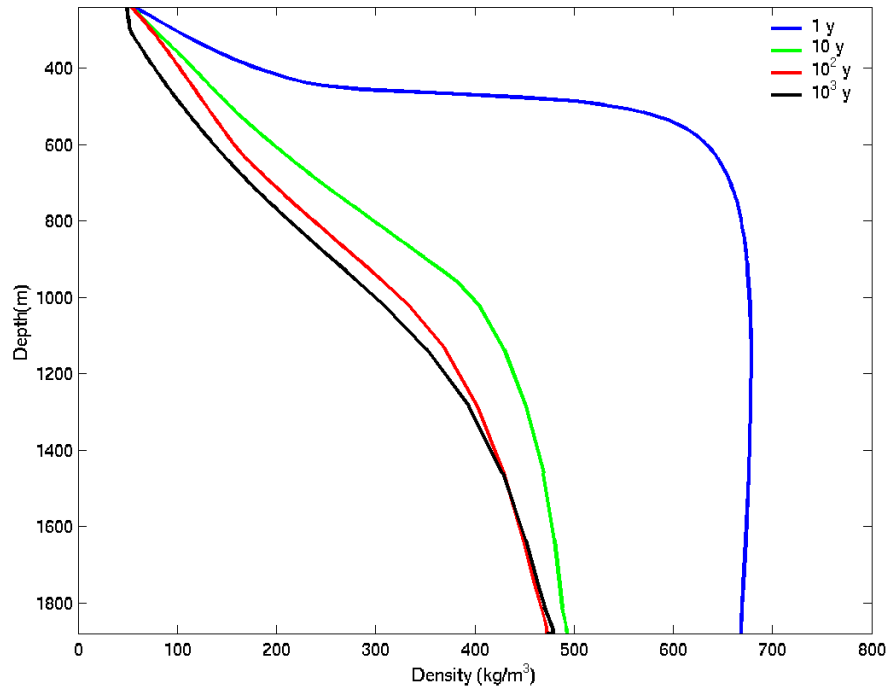


Figure 10: CO₂ density along the fault at different times.

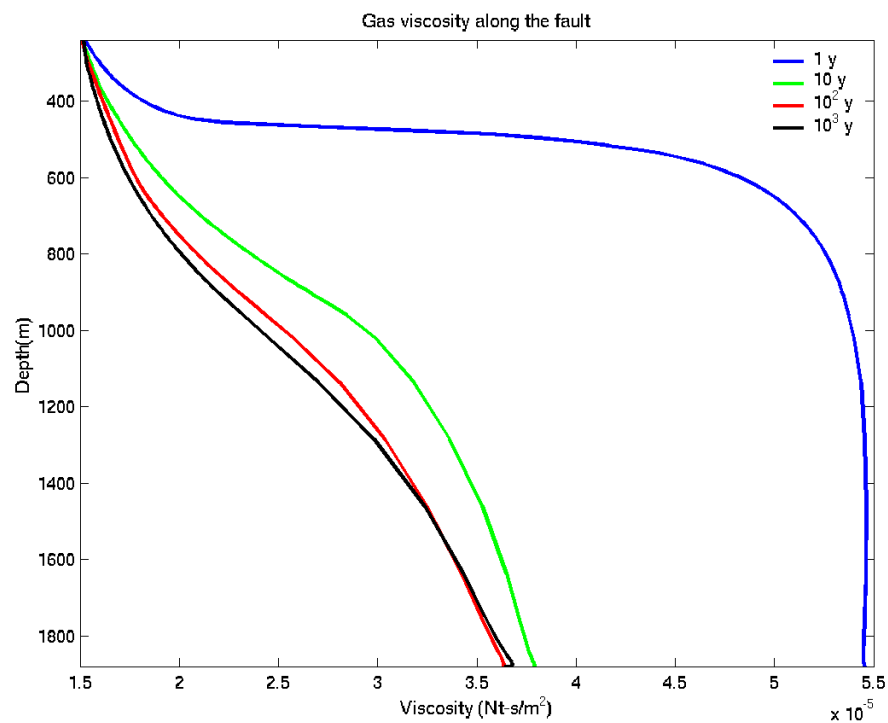


Figure 11: CO₂ viscosity along the fault at different times.

5. SENSITIVITY ANALYSIS OF RESULTS AND UQ ANALYSIS - COUPLED SIMULATION AND EMULATION FOR QUANTIFYING FAULT LEAKAGE

If NUFT models are defined as simulation of physical processes, a reduced-order model (ROM) (also called a response function (surface), an emulation model, or a surrogate model) is a statistical approximation of numerically simulated realizations. The emulated statistical approximation provides higher-dimensional information of possible simulations in parameter space. The following coupled simulation-emulation process was conducted:

1. Data collection for defining ranges of uncertain parameters
2. Sampling in parameter space
3. Model generation and execution
4. Sensitivity analysis and parameter screening
5. Re-define parameter space resulting in new sample points
6. Construction of ROMs using PSUADE
7. Emulation on ROMs to provide leakage statistics

PSUADE was developed by Lawrence Livermore National Laboratory (LLNL) as a code for UQ tasks such as forward uncertainty propagation, qualitative and quantitative sensitivity analysis, parameter exploration, risk analysis, and numerical optimization. It employs the non-intrusive or sampling-based approach to UQ that does not require simulation codes to be modified and ensures that it can easily be integrated with a variety of application simulators. PSUADE is equipped with many response-surface generation and validation techniques. These techniques can be coupled with other UQ techniques such as numerical optimization and Markov Chain Monte Carlo methods for calibration and parameter estimation.

In Steps 2 and 4 the Latin hypercube (McKay et al., 1979) method was used to produce 1,000 sample points, which yielded 865 and 878 successful runs out of 1,000, respectively. Results from Step 4 were used in a Sobol sensitivity analysis to identify the relevant parameters (Figures 12 and 13). Based on this analysis fault permeability was identified as the dominant parameters, allowing the number of variable parameters to be reduced in the refined sampling set (Step 5). Table 3 displays the redefined parameter space. In Step 7, LP-tau (Shukhman, 1994) was used to produce 100,000 sample points using the ROM to produce the necessary statistical output for UQ. The adopted boundary pressure was dependent on distance (using a distance scaling factor) and a pressure-magnitude scaling factor, to reflect the uncertainty on the reservoir pressure, in the equation below:

$$\text{Pressure [Pa]} = P0 * x4 * (-2.2133e-5 * s + 0.9958)$$

This pressure is based on the time-dependent pressure profiles at the fault inlet, where coefficient $x4$ is the scaling factor of boundary pressure in the ROM. A simple saturation curve was used without considering the distance effect, because time-dependent saturation had a minor effect on fault leakage rate. Time-dependent saturation may need to be revisited for the second-generation of risk profiles. Finally, a scaling factor for caprock permeability was used to limit caprock permeability to be less than the permeability of the fault.

Figure 14 and 15 represents CO₂ and brine leakage rates as a function of time derived from the ROM at specific confidence levels. Analytical expressions that capture the range of leakage rates for CO₂ and brine will be incorporated into groundwater simulations to assess the impact of leakage to groundwater chemistry.

Table 3: Data collection, sampling, and refined sampling using most sensitive parameters determined from the Sobol sensitivity analysis

Parameter	Sampling Range		Parameter	Refined Sampling using Most Sensitive Parameters	
	Min	Max		Min	Max
Fault width (m)	0.1	2.0	Distance scale	0.0	1.0
Fault permeability log [m ²]	-14	-12	Fault permeability log [m ²]	10 ⁻¹⁹	10 ⁻¹³
Aquifer permeability log [m ²]	-15	-13	Aquifer permeability log [m ²]	10 ⁻¹⁵	10 ⁻¹³
Cap perm log [m ²]	-19	-17	Cap perm log [m ²]	0.0	1.0
Pressure [Pa]	1.8 ⁷	2.35 ⁷	Pressure [Pa]	0.0	1.0

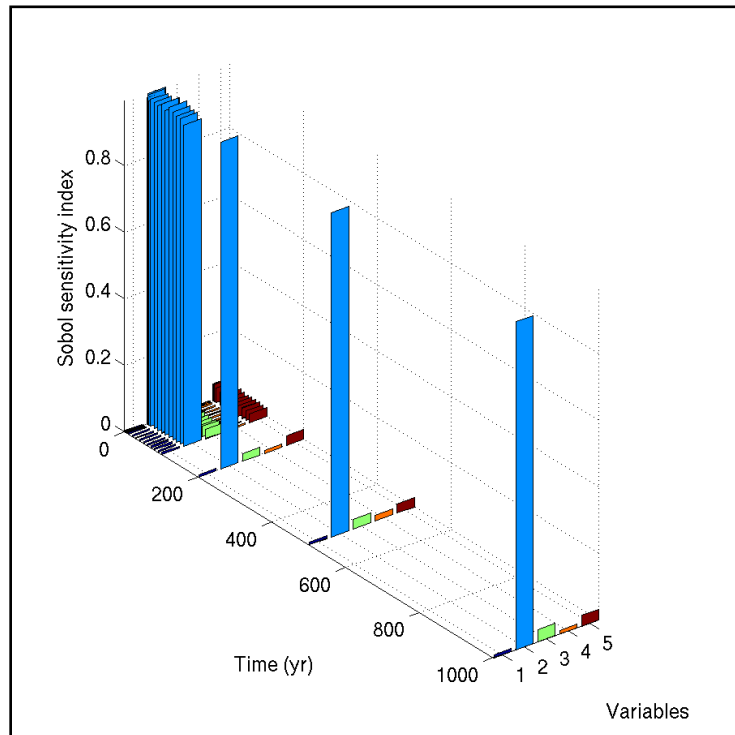


Figure 12: Sobol index.

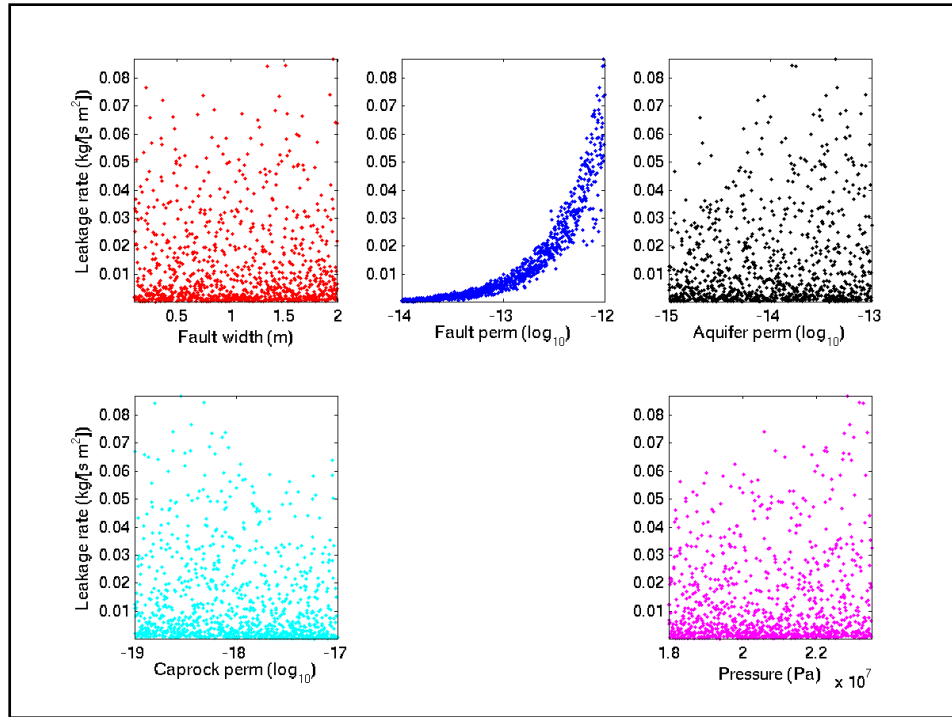


Figure 13: Scatter plots of screened parameters.

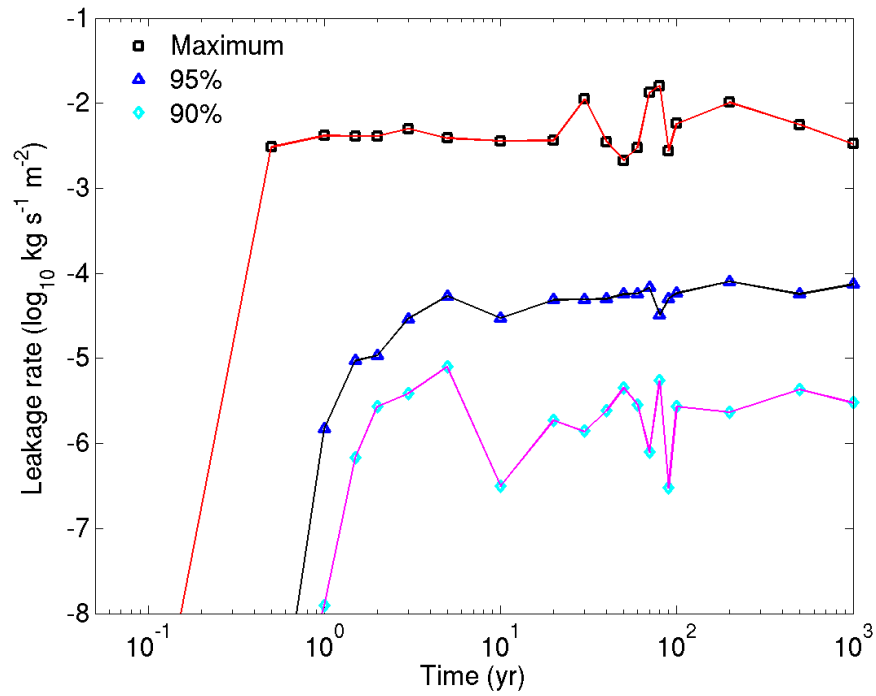


Figure 14: CO₂ leakage rates derived from the ROM at specific confidence levels.

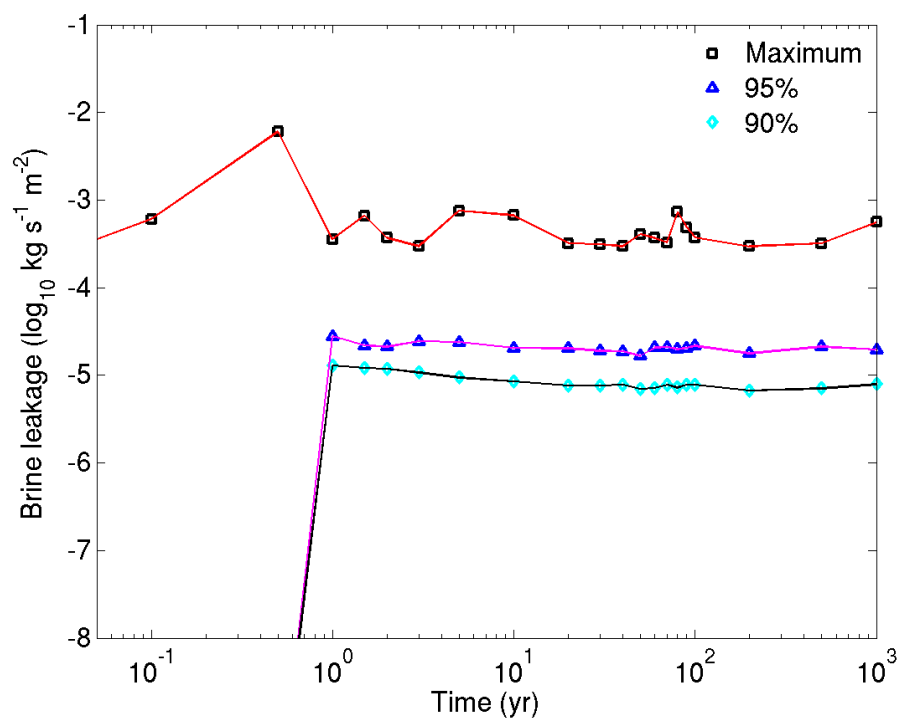


Figure 15: Brine leakage rates derived from the ROM at specific confidence levels.

6. APPLICABILITY AND LIMITATIONS

This ROM was developed to predict the flux of CO₂ and brine from a deep reservoir to a shallow groundwater aquifer. It should be emphasized that the ROM predictions are site specific, and critically depend on the assumed geometry and reservoir boundary conditions. The proposed ROM generation methodology, however, is quite general. To examine a new site, the geometry and reservoir boundary conditions can be modified, and the high-fidelity simulations re-run. A new site-specific ROM can then be constructed from these results.

7. SUMMARY

The fault leakage scenario described in the present document corresponds to CO₂ and brine leakage through a fault, with multiphase and non-isothermal effects, that spans from a CO₂ storage reservoir in *Field A* to an overlying aquifer. Using NUFT 1,000 models were run varying five dimensions: fault permeability, aquifer permeability, scaling factor of caprock permeability, scaling factor of pressure, and scaling factor of distance. A second set of NUFT simulations was run with refined parameter based on the sensitivity analysis of the first set. Response surfaces were then constructed with PSUADE for 19 time steps from 0.5 to 1,000 years as functions of the refined parameter set. On each response surface, 100,000 models were run to generated CO₂ and brine leakage rate profiles for different percentiles.

The current analysis corresponds to the first-generation of leakage risk profiles with the objective to provide leakage rates to the Groundwater Protection Working Group. It has several assumptions and limitations mainly due to its 2-D geometry and the simplistic representation of the fault zone geometry and properties. Furthermore, this model currently does not account for the effect of the in situ stress. All these limitations will be address in further stages of this work.

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NRAP is an initiative within DOE's Office of Fossil Energy and is led by the National Energy Technology Laboratory (NETL). It is a multi-national-lab effort that leverages broad technical capabilities across the DOE complex to develop an integrated science base that can be applied to risk assessment for long-term storage of carbon dioxide (CO₂). NRAP involves five DOE national laboratories: NETL, Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Pacific Northwest National Laboratory (PNNL).

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